Tangent Unit-Vector Fields for Liquid Crystals and Nanoparticles

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We study two model problems concerned with (i) nematic liquid crystal configurations within three-dimensional polyhedral geometries with planar boundary conditions and (ii) monolayer-protected nanoparticles. These seemingly different problems can be mathematically modelled in terms of tangent or planar unit-vector fields. In case (i), we work within the Oseen-Frank theory for nematic liquid crystals and the nematic configuration is modelled by a three-dimensional unit-vector field. The tangent boundary conditions naturally create defects at the polyhedral vertices and we fully characterize the topology of tangent unit-vector fields on polyhedra and compute explicit bounds for their Dirichlet energy in terms of the geometry and topology. In case (ii), we model the tilt-vector of the molecular axes on an octahedral nanoparticle using a Ginzburg-Landau model on the eight facets of the nanoparticle. We describe different tilt configurations (continuous, crystallographic) by means of different boundary-value problems for the Ginzburg-Landau model for the two-dimensional tilt vector and numerically compute a phase diagram for the different allowed configurations in terms of preferred tilt angle, geometry, elastic properties and intermolecular Van der Waals interactions. Our work is an example of how tangent boundary conditions naturally create defects in polyhedral geometries and how defect-stabilized states can offer new possibilities for material design and optimization. This is joint work with Jonathan Robbins, Maxim Zyskin, Chris Newton, Luca Giomi, Mark Bowick and Xu Ma.