MATHEMATICAL MODELS FOR CHROMONIC LIQUID CRYSTALS

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This talk is concerned with a peculiar class of lyotropics: chromonic liquid crystals (CLCs). Chromonics in the nematic phase enjoy the head-tail symmetry, that is, they are non-chiral materials with a tendency for their constitutive elements to bundle together so that a director $\boldsymbol{n}$ can be defined at a mesoscopic scale and lacks polarity. The ground state of ordinary nematic liquid crystals is attained when $\boldsymbol{n}$ is uniform in space, while when CLCs are confined in capillary cylinders with degenerate boundary conditions then they are instead observed to acquire a nonuniform arrangement. In particular, their ground state in a cylindrical capillary, often referred to as the *escaped twist* (ET) field is two-fold; it consists of two symmetric twisted configurations (left- and right-handed), each variant occurring with the same likelihood. Despite their peculiar behaviour in 3D, the Frank theory for nematics has been applied to rationalize the experiments with capillary tubes. This is a variational theory which posits a free-energy density quadratic in the director gradient that penalizes all distortions of $\boldsymbol{n}$ away from a uniform alignment. In particular, in a new alternative form, a *double-twist* distortion is identified and corresponds to the elastic constant $(K_{22} - K_{24})$. Ericksen's inequalities ensure that Frank's energy density is positive definite, and the spontaneous emergence of chirality in the nematic texture is not conceivable when they hold. Thus, as expected, Frank's elastic theory justifies the observed configurations of CLCs under cylindrical confinement only if the relevant Ericksen's inequality, $K_{22} \geq K_{24}$, is violated, and so only if Frank's free-energy functional is unbounded below in $3D$ Euclidean space. The negativity of $(K_{22} - K_{24})$ suggests that the pure double-twisted configuration should be the ground state of CLCs in $3D$ space. Unfortunately, this ideal state is only attainable along a $1D$ curve and its extension to a tubular region introduces by necessity a non-uniform texture with pure double twist only along the axis of the cylinder. This is precisely the ET field experimentally observed for CLCs in cylindrical capillaries subject to degenerate boundary conditions. Taking for granted that the ground state of CLCs is an ideal (unattainable), pure double-twist, we may say that the ET field is actually a 'pseudo-ground state'. The following questions then arise: is anything wrong in applying Frank's elastic theory to these materials? Do we need a new elastic theory for CLCs? It follows from a geometric representation for the energy term K_{24} when $\boldsymbol{n}$ is required to obey planar anchoring conditions on the boundary that even when one of the Ericksen's inequalities involving K_{24} is violated, as in this case, the stored Frank's energy is bounded below. Hence, hardly confining boundary conditions could ensure the existence of the minimum also when the free-energy functional is unbounded below. It can thus be legitimate to apply Frank's theory to this particular class of materials under confinement when $K_{22} < K_{24}$. In particular, the local stability of ET field is established through a general formula for the second variation of the free-energy functional. But, does this really always suffice? Even for free-boundary conditions? To resolve these issues, this talk examines the consequences of the violation of Ericksen's inequality $K_{22} \geq K_{24}$ to ascertain whether they are all harmless. The ultimate conclusion is that Frank's free energy is not apt to describe the elasticity of CLCs because it entails paradoxes that arise if above Ericksen's inequality is violated. This is not only a destructive talk; it also proposes an amendment to the Frank's theory, in the form of a quartic correction to the free-energy density, which promises to reinterpret correctly all experimental findings without leading to any paradox.

This is a joint work with Epifanio G. Virga.

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