## CHAPTER 4. CHIRAL NEMATICS CONFINED IN SPHEROIDS



Figure 4.8. Twist cylinder structure in (left) a droplet ( $\varphi = 1$ ) and (b) a prolate ( $\varphi$ ) with N = 1 and  $W = 1 \times 10^{-4} J/m^2$ . Three concentric cylindric shells indicating different orientations of the director field. (Center) Cross section view of the director field at z = 0. The color map indicates the moleuclar orientation relative to the z-axis: blue is perpendicular and red is parallel.

for a droplet and a prolate. As  $\varphi$  increases, the cylinders follow this stretching in the z direction. If we look at the cross section of the geometry, the outer section follows the boundary condition; the director field twist gradually until it is parallel to the z-axis as we approach the core of the geometry.

For droplets, the orientation of a cholesteric is indistinct. Since the director field is virtually unrestrained, the cholesteric axis of rotation is not strictly aligned with the major axis of the geometry. For geometries with  $\varphi \neq 1$  the cholesteric axis showed tilting without a preferred angle.

For this particular case, simulations starting from two different ansatze (uniaxial and twist cylinder) were performed for four different geometries ( $\varphi = 0.5, 1.1, 1.3, 1.5$ ), and two chiralities (N = 0.5, 1). The ansatze were rotated an angle  $\theta$  respect to the *z*-axis. Figure 4.9 shows the total free energy for a prolate ( $\varphi = 1.5$ ) in the low chirality regime as well as the final configurations of a rotated TC with N = 1. The total free energy does not fluctuate considerably since all final configurations show a free energy of the same order of magnitude. This behavior is noted in the bulk and elastic contributions. The only resistance to the orientation of the cholesteric is in the surface free energy (not shown) with a difference of  $200 k_B T$ , but this effect is unperceived. Although energetically there is no difference, a distortion of the TC occurs as the inclination approaches the minor axis of the geometry. This is evidenced by the torsion of the region parallel to the surface of the prolate (in red) as  $\theta$  approaches  $90^{\circ}$  showing a slight resemblance to a lemniscate. The patterns of the surface contours are typical of a cholesteric as reported in [91], whereas a final configuration with  $\theta = 0$  is similar to a uniaxial phase where the parallel regions form a perfect ring in the equator of the geometry.