Simulating defect structures in nematic liquid crystal shells

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Recent theoretical and experimental studies have investigated the textures of nematic liquid crystals confined to a shell geometry between two spheres. When the shell is very thin, the structure becomes effectively two-dimensional, and provides an experimental realization of nematic order and defects in a curved geometry. As the shell becomes thicker, the behavior crosses over to a three-dimensional liquid crystal, with different types of defects.

To study this dimensional crossover, we perform simulations of nematic order in a shell geometry. For these simulations, we use a disordered lattice, or mesh, constructed through random sequential adsorption on the inner surface, the outer surface, and within the bulk of the shell. A nematic director is placed on each site of the mesh, and the directors interact with their neighbors through an $(n_i \cdot n_j)^2$ interaction. By minimizing the energy, we determine the nematic texture as a function of the radii and thickness of the shell, and as a function of the off-center displacement of the inner sphere. The results demonstrate a variety of different structures: a new equilibrium state with two vortex lines and one boojum pair, as well as the previously predicted four vortex line defect structure, and a two boojum pair defect structure that occurs rarely. We find that these structures are observed in the experiment and computer simulations at the same conditions, because their energies are approximately equal. Also, we observe a complex evolution of the structures as the inner sphere moves off-center. By calculating the energy change during such motion, we determine that there is little or no elastic force acting on the inner sphere, and hence the experimental motion of the inner sphere must be due to gravitational rather than elastic force.