Supplementary information: Stability of chiral crystal phase and breakdown of cholesteric phase in mixtures of active-passive chiral rods

Jayeeta Chattopadhyay, Jaydeep Mandal, Prabal K. Maiti

January 30, 2024

1 Absence of ordered phases without wall



Figure A1: Representation of the configurations obtained for a system of chiral particles with p = 6.67D (the value of D is taken to be 1.0), showing a) Isotropic phase (I) at low pressure $P^* = 0.1$, and b) c) d) jammed state at pressure $P^* = 0.5, 0.8$ and 1.2 respectively. The pressure is expressed in reduced units $P^* = \frac{P}{k_B T}$

Simulating the system of soft helical rods with periodic boundary conditions exhibits jammed state at high densities, although the low density isotropic phases is observed in the system. In order to avoid the jammed state, we have used walls in our simulations, that help in the formation of the cholesteric phase within the simulation timescale, by offering an homeotropic alignment to the particles. Fig A1 shows the snapshots of such jammed states at different pressures.

2 Breakdown of Cholesteric phase



Figure A2: For molecular pitch p = 9.92D: a) The final configuration of the system at $\chi = 5$, the cold particles form ordered smectic phase near the walls, whereas the hot particles form the isotropic phase at the interior. b) The variation of $Cos(\theta)$ with x for the same system. The regions near the wall show lesser fluctuation in the value of $Cos(\theta)$ due to smectic ordering, whereas isotropic region shows larger fluctuation. Also the overall variation of $Cos(\theta)$ doesnot show the behaviour typical to cholesteric phase, indicating the breakdown of the initial cholesteric phase.

Starting from an equilibrated cholesteric phase for a system of soft helix of microscopic pitch p = 9.92 at reduced pressure $P^* = 0.9$, we use the two temperature model to observe the fate of the cholesteric phase. Phase separation between the hot and cold particles takes place. Our results show that when activity is introduced, the hot particles form an isotropic phase while the cold particles exhibit an ordered phase that is shown to be smectic in the observed range of activities. Therefore the initial cholesteric phase is breaking down under the influence of temperature difference.