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A helical fluid in confined quasi-one-dimensional hard spheres

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Hard spheres confined to long, narrow, cylindrical channels spontaneously form helical structures. We use molecular dynamics simulation to show that the thermodynamics, structure and dynamics of these systems are dominated by the presence of topological defects that reverse the local twist direction of the helix. The equilibrium fluid exhibits two heat capacity maxima related to structural crossovers associated with the onset of helix formation at low densities and a Schottky-like anomaly caused by the rapid elimination of defects at high density. As expected, the fluid remains achiral over the densities studied. Structural relaxation in the system occurs through the creation, diffusion and elimination of the defects, which leads to a stretched exponential decay in the local twist auto-correlation function and a fragile-strong fluid crossover located at the high density heat capacity maximum. However, introducing excess helical twist into the system leads to the formation of a chiral fluid characterized by the presence of loosely bound defect pairs which become more tightly bound with increasing excess helical twist. The local twist auto-correlation function in the chiral fluid decays as a power law at long times while the translational correlation function decays exponentially like a fluid.

Keyword-1

chiral fluid

Keyword-2

hard spheres

Keyword-3

molecular dynamics simulation

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