How the number of vertices determines the thermodynamics of hard polygon fluids

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Everywhere around us, shape plays a key role in dictating emergent behavior and physical phenomena. For instance, aerodynamic vehicle design relies on geometric optimization to reduce drag, liquid-crystal displays exploit phase behavior dictated by particle anisotropy, and the curved walls of concert halls are engineered to direct sound. Naturally, shape also plays an important role in fluids, where the macroscopic properties of a system are influenced not only by thermodynamic variables such as temperature, volume, and particle number, but also by the characteristics of its constituents.

This raises a central question: How do the geometric features of hard bodies influence thermodynamic behavior? To address this, we perform extensive two-dimensional Monte Carlo simulations of fluids composed of various polygons with k vertices, as well as deformations of a disk corresponding to the limit of infinite vertices in the isotropic phase. We find that the equations of state for the pressure, expressed as functions of the packing fraction, collapse into narrow, well-defined bands that are uniquely determined by the number of vertices k, provided that all polygons represent only moderate deformations of their regular counterparts. This collapse indicates that regular polygons act as local minima of the free energy with respect to small variations in particle shape. We support this observation analytically by showing that the thermodynamics of slightly deformed polygons is accurately approximated by that of a fluid composed of regular polygons with the same area and the same number of vertices. We also find that the emergent bands exhibit a clear ordering: the fluid's pressure decreases systematically with increasing number of vertices, approaching the hard-disk equation of state in the limit of infinite vertices. This ordering becomes increasingly pronounced as the magnitude of the deformation decreases.

Our results establish a geometric framework for predicting fluid behavior across the full density range of the isotropic phase. The emergence of distinct, shape-dependent thermodynamic bands challenges the conventional expectation of a universal equation of state for hard-particle fluids. Moreover, the strong correlation between the equation of state and the number of vertices suggests a practical route for inferring particle shape information directly from pressure measurements. Together, these findings highlight the deep and quantifiable role of geometry in governing the thermodynamics of hard-particle systems.