

Thermodynamic Properties of the Gaussian Core Model Fluid from Molecular Dynamics

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During the past decade there has been considerable interest in the ability of soft bounded potentials to describe properties of condensed matter. For example, soft bounded potentials provide a reliable qualitative description of the thermal behavior of globular polymers or molecular aggregates such as micelles, which can be modelled as soft inherently interpenetrable “particles.” One of the most natural soft bounded potential in statistical mechanics is the Gaussian core model (GCM) introduced by Stillinger.¹ The GCM fluid exhibits density and structural anomalies as well as other water-like anomalies associated with re-entrant melting behavior. Equilibrium transport properties of the GCM fluid such as the self-diffusion coefficient and the shear viscosity also show anomalous behavior,² resulting in the violation of the Stokes-Einstein relation. Other properties such as the energy³ and the pressure as well as the viscosity in sheared non-equilibrium fluid states also show unusual behavior. Despite recent progress, the thermodynamic properties of the GCM are far from being completely understood and the occurrence of a whole range of anomalous properties suggest that the GCM possesses unexplored anomalies similar to water, which might have implications for a broad range of water-like potentials. In this work, molecular dynamic simulation results are reported for the pressure, energy, isothermal pressure coefficient, thermal expansion coefficient, isothermal and adiabatic compressibilities, isobaric and isochoric heat capacities, Joule-Thomson coefficient and speed of sound of the Gaussian Core Model for a wide range of state points.³ These properties were obtained using the treatment of Lustig^{4,5} whereby thermodynamic state variables are expressible in terms of phase-space functions determined directly from molecular-dynamics simulations. The results show that the Gaussian Core model shares many of the anomalies commonly associated with water such as a pressure minimum (density maximum), a negative thermal expansion coefficient, and a minimum isobaric heat capacity.

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