Thermodynamic Properties of the Gaussian Core Model – Fluid

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The Gaussian Core Model (GCM) is a core-softened potential that was first introduced nearly 30 years ago. The potential is bounded, i.e. a full overlap between particles is possible. This can be a realistic situation, e.g. in polymer solutions between polymer chains. Polymer chains are soft, interpenetrable entities. In this context, the GCM became very popular in the field of soft condensed matter physics. Moreover, the phase diagram of the GCM displays unusual features, such as re-entrant melting and a maximum freezing temperature. Using a decorated modification of the GCM, inverse melting could be modeled by this potential.

Because of this large interest in the GCM, a description of the thermodynamic properties of the liquid phase is desirable. Using intensive Monte Carlo simulations, we develop an analytical equation of state for a very large density and temperature range. We derive response functions, such as the isothermal compressibility, the thermal expansion coefficient, and the heat capacity. We can show that all three properties behave anomalously, similar to water. The temperature and density dependence of the fluid structure is studied by means of the pair correlation function and the structure factor. At low densities, the system behaves like a simple liquid: spatial overlapping of particles is highly improbable. When the density is increased, overlapping of particles occurs. Using the pair correlation function, we can analyze the change between ‘singled’ and ‘doubled’ local configurations. We show that the onset of doubling begins at a dimensionless density of about 0.35. For very high densities, the GCM system loses its structure as it approaches the so called ‘infinite-density ideal gas limit’.