Thermodynamic, dynamic and structural properties of the hard sphere systems revisited by molecular dynamics simulation

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New developments in determination of physical properties of the hard sphere (HS) systems will be presented. Some aspects of the simulation methods used in the calculations will be mentioned.

In the first part of the talk thermodynamic and dynamical properties of the monocomponent HS system obtained from extensive molecular dynamic calculations carried out with large system sizes (number of particles, N) and long times, will be discussed. An accurate compressibility factor of the HS solid and fluid branches will be given. Comprehensive representations of the HS self-diffusion coefficient, shear viscosity and thermal conductivity will be presented and a comparison with the corresponding Enskog theory expressions will be discussed.

In the second part of the presentation a novel approach to obtain structural properties of additive binary hard-sphere mixtures will be presented. The method combines accurate molecular dynamics simulation data, the pole structure representation of the total correlation functions, and the Ornstein Zernike equation. A comparison of the obtained direct correlation functions with those predicted with the Percus-Yevick and Rational-Function Approximation (RFA) methods will be done. Some advantages of the RFA approach will be indicated.