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Thermodynamic properties of molecular fluid mixtures of hard ellipsoids

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Abstract. Thermodynamic properties of molecular fluid mixtures of hard ellipsoids are calculated. Numerical results are given for equation of state and excess-free energy of the binary mixture of both additive and non-additive hard ellipsoids. It is found that the equation of state and free energy of mixtures increase with increase of anisotropy parameter χ_0.

Keywords. Hard ellipsoid; equation of state; excess free energy; anisotropy; binary mixture.

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1. Introduction

This paper is concerned with the evaluation of thermodynamic properties of a molecular fluid mixture, whose molecules interact via hard ellipsoid potential. We consider the case where the constituent molecules have the same length to width ratio χ_0.

Many theoretical attempts such as van der Waals one- and two-fluid theories (Leland *et al* 1968; Henderson and Leonard 1971a, b) and perturbation theory (Henderson and Barker 1968; Smith 1971; Smith and Henderson 1972) have been made to understand the structural and thermodynamic properties of simple atomic fluid mixture of hard spheres, where the length-to-width ratio χ_0 is unity. The basis of the perturbation theory is to expand the properties of a hard sphere mixture about that of a one-component fluid of hard spheres of diameter d_0 in power of $(d_{\alpha\gamma}^n - d_0^n)$. It is found that the first order perturbation theory becomes identical to the van der Waals one-fluid (vdW 1) theory, when $n = 3$ (Smith and Henderson 1972; Adams and McDonald 1975) and gives good results for the thermodynamic properties (Smith 1971; Henderson and Leonard 1971b). This method can be extended to the molecular fluid mixture of hard ellipsoids.

In this paper, we examine the theory for a molecular binary mixture of hard ellipsoids and calculate the thermodynamic properties of the system. In § 2, we discuss the theory for calculating the thermodynamic properties of a binary mixture of hard ellipsoids.

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