Calculation of the pressure and interfacial tension of confined hard-spherocylinders fluids by volume perturbations

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A method to determine the components of the pressure tensor for fluids of purely repulsive molecules is presented. This volume perturbation approach is valid for convex and non-convex molecules alike, and accounts for the asymmetry of expansive and compressive contributions to the pressure tensor. When applied to a confined system of liquid crystals, represented as hard-spherocylinders, one may calculate the pressure components tangential and normal to the confining surfaces. From these we may obtain predictions for the interfacial tension of the isotropic phase and the more challenging case of the higher density nematic phase. This work helps demonstrates the potential of perturbation methods.