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Improved hard sphere radial distribution function in the CRIS equation of state model[1] BENJAMIN COWEN, JOHN CARPENTER, Sandia National Laboratories — Experiments and theory have been refined for decades in order to better approximate thermodynamic properties of materials. These thermodynamic properties are stored in equation of state (EOS) models, and used as input, such as SESAME tables, into higher level shock physics codes. To ensure the integrity of these codes, the accuracy of the EOS models is paramount. The CRIS (Corrected Rigid Spheres) EOS model [1], developed from fluid perturbation theory using a hard sphere reference system, has been successfully used to calculate the EOS of many materials, including gases and metals. The hard sphere radial distribution function (RDF) plays a pivotal role in choosing the hard sphere diameter, through a variational principle, as well as the thermodynamic response. Despite its success, the CRIS model has some shortcomings in that it predicts too large a temperature for liquid-vapor critical points, and breaks down at large compression. To remedy these limitations, we demonstrate the effects of an improved analytical representation of the RDF. [1] G. I. Kerley, J. Chem. Phys. 73, 478 (1980).

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